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First-principles calculations of the amplitudes of the electron transition from a ligand to the 5d shell of Yb3+: KZnF3

Anikeenok O.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The expressions describing the amplitudes of a transition of an electron from a ligand to vacant shells of the central ion of an impurity center are derived. The amplitudes of a transition of an electron from a ligand to the 5d shell of a rare-earth ion are calculated from first principles. The calculations are performed in the basis set of orbitals taken in the form of 5s, 5p, 4f, 5d, and 6s electron shells of the central ion and 2s and 2p electron shells of the ligands. No expansion in terms of overlap integrals is employed in the calculations. The matrix elements of the (I + S)-1 matrix are determined in the chosen basis set of orbitals. The amplitudes thus calculated are in good agreement with those obtained by fitting of the experimental data. © Nauka/Interperiodica 2006.

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